

Access DB# 95575

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: DAWN GARRETT Examiner #: 76107 Date: 6/2/2003
Art Unit: 1774 Phone Number 305-0788 Serial Number: 101086067
Mail Box and Bldg/Room Location: _____ Results Format Preferred (circle): PAPER DISK E-MAIL

CP3-1703 8B32

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: ORGANIC ELEMENT FOR ELECTROLUMINESCENT DEVICES

Inventors (please provide full names): _____

BENJAMIN P. HOAG, DENIS Y. KONDAKOVEarliest Priority Filing Date: 2/28/2002

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search a light-emitting device
Containing a light-emitting layer where the dopant
is a boron compound containing a bis(azinyl)methylene boron
Complex group.

Also search specifically:
claim 4 compound, claim 5 compound,
and Formula (1) compounds found in claim 14

See attached claims.

STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: <u>EA</u>	NA Sequence (#) _____	STN <u>\$158.05</u>
Searcher Phone #: _____	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) <u>(2)</u>	Questel/Orbit _____
Date Searcher Picked Up: _____	Bibliographic _____	Dr.Link _____
Date Completed: <u>6-4-03</u>	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: <u>10</u>	Fulltext _____	Sequence Systems _____
Clerical Prep Time: _____	Patent Family _____	WWW/Internet _____

What is claimed is:

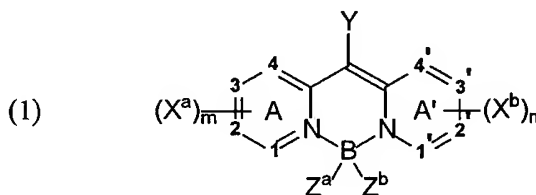
1. An OLED device comprising a light-emitting layer containing a host and a dopant where the dopant comprises a boron compound containing a bis(azinyl)methene boron complex group.
2. The device of claim 1 wherein the layer comprises a host and dopant where the dopant is present in an amount of up to 10 wt % of the host.
3. The device of claim 2 wherein the dopant is present in an amount of 0.1-5.0 wt % of the host.
4. The device of claim 1 wherein the boron complex group is a 6,6,6-tricyclic bis(azinyl)methene boron complex group.
5. The device of claim 4 wherein the boron complex group is a bis(pyridinyl)methene boron complex group.
6. The device of claim 5 wherein at least one of the pyridyl groups is substituted.
7. The device of claim 6 wherein at least one of the pyridyl groups has substituent groups joined to form a fused ring.
8. The device of claim 1 wherein the host comprises a chelated oxinoid compound or an anthracene compound.
9. The device of claim 8 wherein the host comprises a chelated oxinoid compound.
10. The device of claim 8 wherein the host comprises an anthracene compound.

11. The device of claim 1 wherein the host comprises tris(8-quinolinolato)aluminum (III) or 2-*tert*-butyl-9,10-di-(2-naphthyl)anthracene.

12. The device of claim 1 wherein the substituents are selected to provide an emitted light having a green hue.

13. The device of claim 1 wherein the substituents are selected to provide a reduced loss of initial luminance compared to the device containing no boron compound of claim 1.

14. The device of claim 1 wherein the dopant compound is represented by Formula (1):



wherein

A and A' represent independent azine ring systems corresponding to 6-membered aromatic ring systems containing at least one nitrogen;

each X^a and X^b is an independently selected substituent, two of which may join to form a fused ring to A or A';

m and n are independently 0 to 4 ;

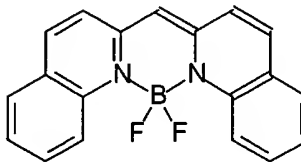
Y is H or a substituent;

Z^a and Z^b are independently selected substituents;

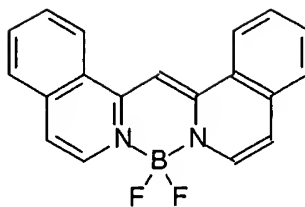
1, 2, 3, 4, 1', 2', 3', and 4' are independently selected as either carbon or nitrogen atoms.

15. The device of claim 14 wherein 1, 2, 3, 4, 1', 2', 3', and 4' are all carbon atoms.
16. The device of claim 14 wherein at least one of ring A or A' contains substituents joined to form a fused ring.
17. The device of claim 14 wherein both ring A and A' contain substituents joined to form a fused ring.
18. The device of claim 14 wherein there is present at least one X^a or X^b group selected from the group consisting of halide and alkyl, aryl, alkoxy, and aryloxy groups.
19. The device of claim 14 wherein Z^a and Z^b are independently selected from the group consisting of fluorine and alkyl, aryl, alkoxy and aryloxy groups.
20. The device of claim 19 wherein Z^a and Z^b are F.
21. The device of claim 14 wherein the layer comprises a host and dopant where the dopant is present in an amount of up to 10 wt % of the host.
22. The device of claim 21 wherein the dopant is present in an amount of 0.1-5.0 wt % of the host.
23. The device of claim 1 wherein the boron compound is selected from the following.

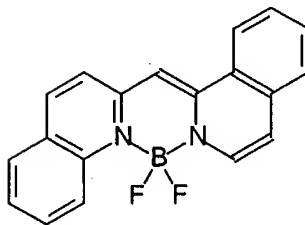
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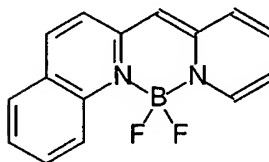
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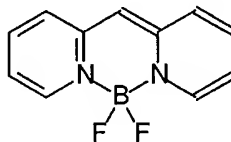
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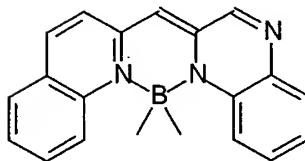
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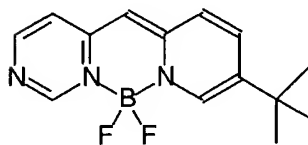
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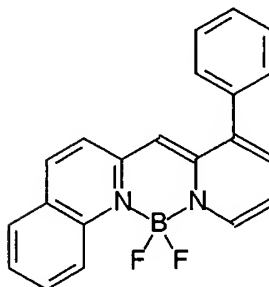
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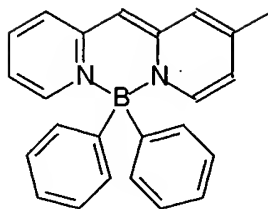
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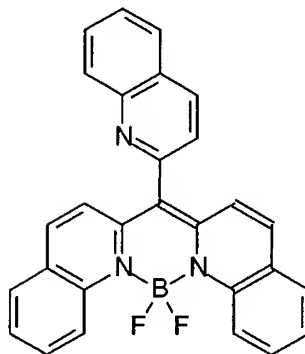
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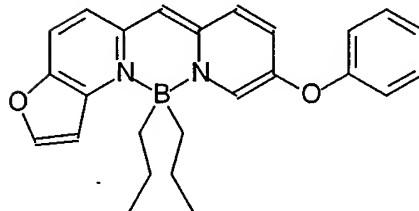
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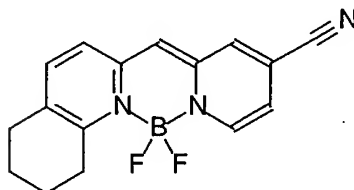
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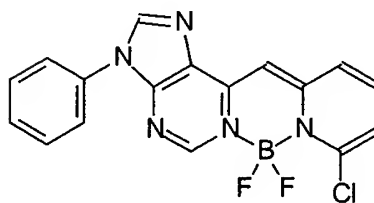
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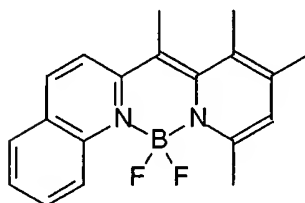
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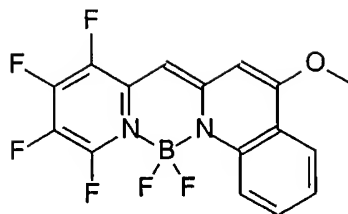
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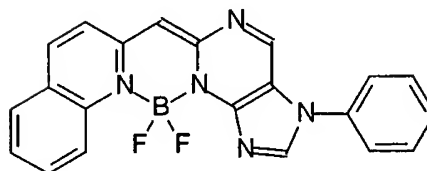
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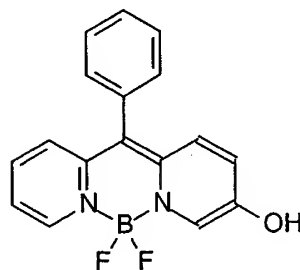
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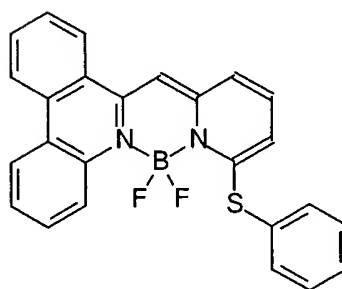
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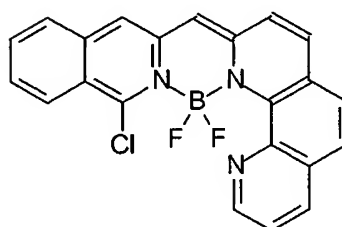
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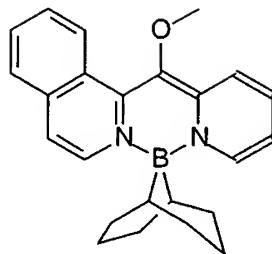
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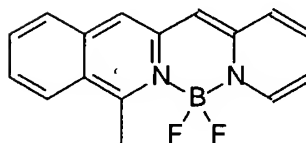
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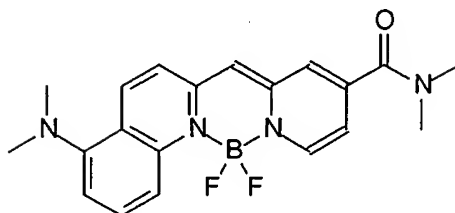
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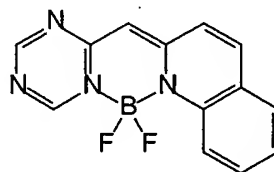
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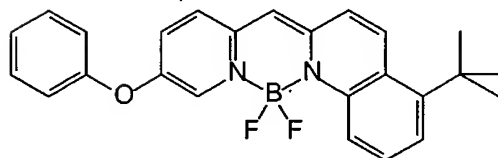
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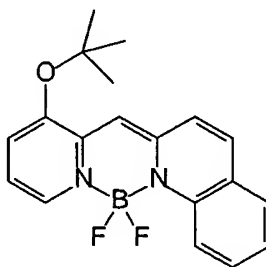
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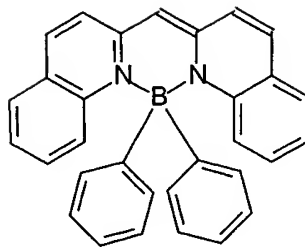
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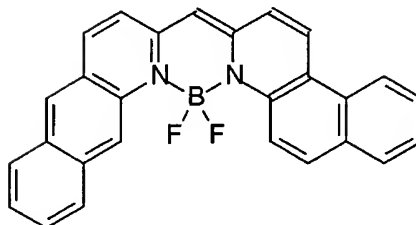
Inv-25



Inv-26

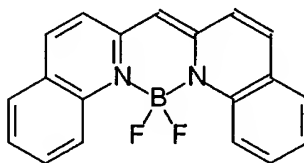


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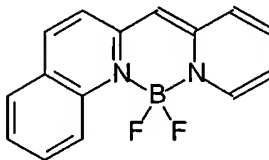


24. The device of claim 1 wherein the boron compound is selected from the following.

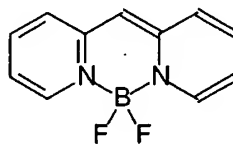
Inv-1



Inv-4



Inv-5



25. A light emitting device containing the OLED device of claim 1.

26. A method of emitting light comprising subjecting the device of claim 1 to an applied voltage.

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STR

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STR L1

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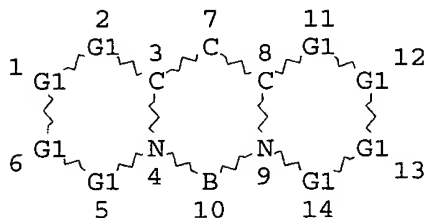
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6 S L5

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L9 6 S L3 FUL

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L3 STR



VAR G1=C/N

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
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10 ANSWERS

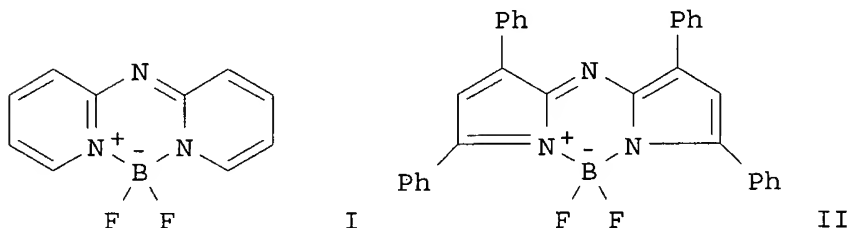
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L7 ANSWER 1 OF 6 ZCAPLUS COPYRIGHT 2003 ACS
1994:682305 Document No. 121:282305 Fluorescent tricyclic
.beta.-azavinamidine-BF₂ complexes. Sathyamoorthi, Govindarao;
Soong, Mou Ling; Ross, Timothy W.; Boyer, Joseph H. (Dep. Chem.,
Univ. New Orleans, New Orleans, LA, 70148, USA). Heteroatom
Chemistry, 4(6), 603-8 (English) 1993. CODEN: HETCE8. ISSN:
1042-7163.

GI



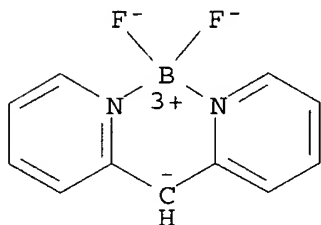
AB Boron trifluoride reacted with 2,2'-dipyridylamine and its N-Me and 6,6'-dimethyl derivs. and 3,3',5,5'-tetraphenyl-6-azapyrromethene to give fluorescent .beta.-azavinamidine (1,3,5-triazapenta-1,3-diene) dyes: 10-azapyridomethene-BF₂ complex (I) (.lambda.f 422 nm, .lambda.las 426 nm), its quaternary 10-Me tetrafluoroborate and 4,6-di-Me derivs. (.lambda.f 362 and 416 nm, resp.), and 1,3,5,7-tetraphenyl-8-azapyrromethene-BF₂ complex (II) (.lambda.f 696 nm). Treating 3,3',4,4'-tetraphenyl-5,5',6-trimethylpyrromethene (prepd. in situ from Et 3,4-diphenyl-5-methylpyrrole-2-carboxylate and acetyl chloride) with BF₃ gave

1,2,6,7-tetraphenyl-3,5,8-trimethylpyrromethene-BF₂ complex.
Absorption for the vinamidine chromophore differed from that for the .beta.-azavinamidine chromophore by a hypsochromic shift of 86 nm in a comparison of a pyridomethene-BF₂ complex with its 10-aza deriv. I and by a bathochromic shift of 105 nm in a comparison of a pyrromethene-BF₂ complex with the 8-azapyrromethene-BF₂ complex II.

IT 42029-62-9P
(prepn. of fluorescent tricyclic .beta.-azavinamidine-fluoroboron complexes)

RN 42029-62-9 ZCAPLUS

CN Boron, difluoro[[2,2'-methylenebis(pyridinato)] (1-)-N,N']-, (T-4)- (9CI) (CA INDEX NAME)



IT 42029-62-9P
(prepn. of fluorescent tricyclic .beta.-azavinamidine-fluoroboron complexes)

L7 ANSWER 2 OF 6 ZCAPLUS COPYRIGHT 2003 ACS

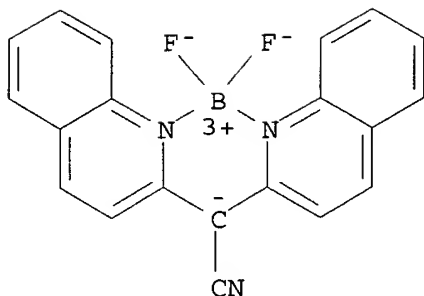
1991:481962 Document No. 115:81962 On the distribution of reactive barriers in disordered materials. Schellenberg, P.; Friedrich, J.; Daltrozso, E. (Inst. Phys. Chem., Johannes Gutenberg-Univ., Mainz, D-6500, Germany). Journal of Chemical Physics, 95(1), 189-94 (English) 1991. CODEN: JCPSA6. ISSN: 0021-9606.

AB The hole-burning photoreaction of a dye complex in alc. glass which undergoes both photochem. and photophys. transformations was studied. Measuring sep. the disappearance of the photoproduct at the resp. wavelength ranges under thermal cycling conditions showed that the photochem. transformed species recovered according to a Gaussian distribution of barrier heights, whereas the photophys. transformed species recovered in accordance with a 1/.sqrt(V) distribution. This behavior is rather general and is intimately related to the nature of the phototransformation process.

IT 73681-66-0
(photochem. hole burning photoreaction of, in alc. glass)

RN 73681-66-0 ZCAPLUS

CN Boron, difluoro(.alpha.-2-quinolinyl-2-quinolineacetonitrilato)-, (T-4)- (9CI) (CA INDEX NAME)



IT 73681-66-0

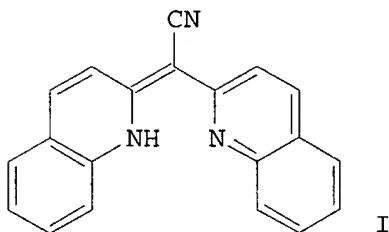
(photochem. hole burning photoreaction of, in alc. glass)

L7 ANSWER 3 OF 6 ZCAPLUS COPYRIGHT 2003 ACS

1980:214409 Document No. 92:214409 The influence of viscosity on fluorescence-quantum yields of a polymethine dye

diquinolinylnylcyanomethane. Griebel, R. (Fak. Chem., Univ. Konstanz, Konstanz, 7750, Fed. Rep. Ger.). Berichte der Bunsen-Gesellschaft, 84(1), 84-91 (English) 1980. CODEN: BBPCAX. ISSN: 0005-9021.

GI



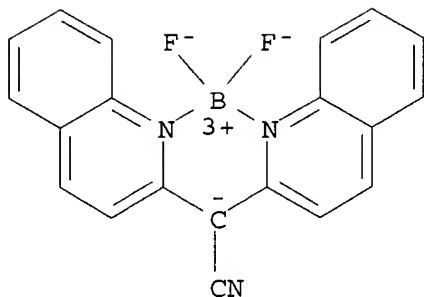
AB The fluorescence-quantum yield of the title compd. (I) depended on the viscosity (temp.). This dependence was explained by coupling of the dominant and viscosity-dependent relaxation mode to an intramol. H/D bridge potential..

IT 73681-66-0

(fluorescence of)

RN 73681-66-0 ZCAPLUS

CN Boron, difluoro(.alpha.-2-quinolinylnyl-2-quinolineacetonitrilato)-, (T-4) - (9CI) (CA INDEX NAME)



IT 73681-66-0
(fluorescence of)

✓ ordered

L7 ANSWER 4 OF 6 ZCAPLUS COPYRIGHT 2003 ACS

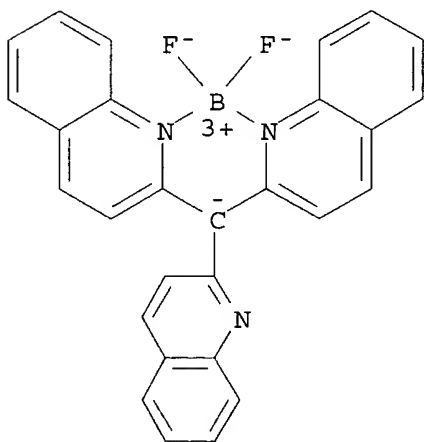
1974:419043 Document No. 81:19043 New laser dyes. Basting, D.; Schaefer, F. P.; Steyer, B. (Max-Planck-Inst. Biophys. Chem., Goettingen, Fed. Rep. Ger.). Applied Physics (Berlin), 3(1), 81-8 (English) 1974. CODEN: APHYCC. ISSN: 0340-3793.

AB A list of 73 new laser dyes is given. These dyes were obtained in screening fluorescent dyes from a dye collection using a powerful N laser of 1 MW peak power and 2.5 nsec pulse width.

IT 53217-34-8
(laser dye)

RN 53217-34-8 ZCAPLUS

CN Boron, difluoro[2,2',2''-methylidynetris[quinolinato] (1-)-N,N']-, (T-4)- (9CI) (CA INDEX NAME)



IT 53217-34-8
(laser dye)

L7 ANSWER 5 OF 6 ZCAPLUS COPYRIGHT 2003 ACS

1973:418682 Document No. 79:18682 Diazaboracyclic cations. III. Homomorph of 9,10-dihydroanthracene. Douglass, James E.; Barelski, Paul M.; Blankenship, Robert M. (Dep. Chem., Marshall Univ., Huntington, WV, USA). Journal of Heterocyclic Chemistry, 10(2), 255-7 (English) 1973. CODEN: JHTCAD. ISSN: 0022-152X.

GI For diagram(s), see printed CA Issue.

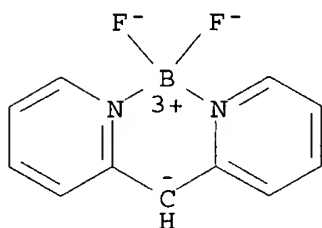
AB The pyridodiazaborine I was prepd. by thermally cyclizing 2,2'-dipyridylmethane.2HBF₄ in the presence of NaBH₄, probably via II (R = F, X = BF₄). I is air-stable but readily cleaved by acid or base; attempts to dehydrofluorinate to give an anthracene homolog failed. II (R = H; X = PF₆, iodide) were also prepd. from I or from the dipyridylmethane.

IT 42029-62-9P

(prepn. and salt formation with fluoroboric acid)

RN 42029-62-9 ZCAPLUS

CN Boron, difluoro[[2,2'-methylenebis(pyridinato)](1-)-N,N']-, (T-4)-(9CI) (CA INDEX NAME)



IT 42029-63-0P 42029-64-1P 42029-65-2P
(prepn. of)

RN 42029-63-0 ZCAPLUS

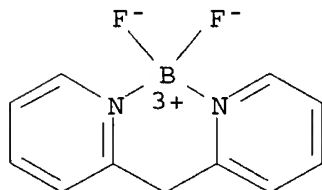
CN Boron(1+), difluoro[2,2'-methylenebis(pyridine)-N,N']-, (T-4)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

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CRN 48153-22-6

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CCI CCS

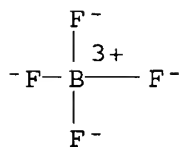


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CRN 14874-70-5

CMF B F4

CCI CCS



RN 42029-64-1 ZCAPLUS

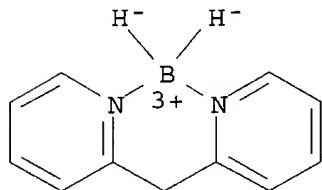
CN Boron(1+), difluoro[2,2'-methylenebis(pyridine)-N,N']-, (T-4)-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 48153-23-7

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CCI CCS

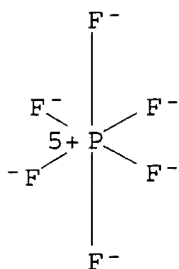


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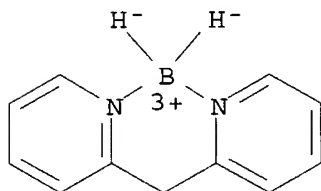
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CCI CCS



RN 42029-65-2 ZCAPLUS

CN Boron(1+), dihydro[2,2'-methylenebis[pyridine]-N,N']-, iodide,
(T-4)- (9CI) (CA INDEX NAME)



● I-

IT 42029-62-9P

(prepn. and salt formation with fluoroboric acid)

IT 42029-63-0P 42029-64-1P 42029-65-2P

(prepn. of)

L7 ANSWER 6 OF 6 ZCAPLUS COPYRIGHT 2003 ACS

1969:434795 Document No. 71:34795 Franck-Condon principle and the light absorption of merocyanines. Scheibe, Guenter; Daltrozzi, E.; Woerz, O.; Heiss, J. (Tech. Hochsch., Munich, Fed. Rep. Ger.). Zeitschrift fuer Physikalische Chemie (Muenchen, Germany), 64(1-4), 97-114 (German) 1969. CODEN: ZPCFAX. ISSN: 0044-3336.

AB In open-chain cyanines (polymethines) the intensity ratio of 0 .fwdarw. 0', 0 .fwdarw. 1', 0 .fwdarw. 2' vibrational bands of the longest-wave electron transition is independent of the chain length. If this fact is explained by assuming that the distance of the potential curve min. between ground and excited state becomes smaller with increasing chain length, good conformity is found with the "extensions" which are obtained by L.C.A.O.-M.O. calcns. (Hueckel M.O. and Pople-Pariser-Parr approxn.). In merocyanines (polyenes), considerably greater "extensions" result in the

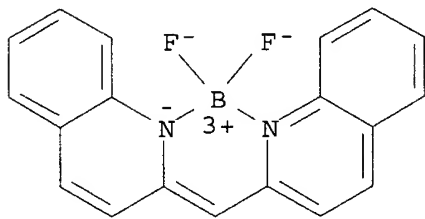
application of the Franck-Condon principle due to the comparatively strong intensity shift towards higher vibrational transitions. If no vibrational structure can be observed in the electron spectrum, the absorption max. of the enveloping curve may appear at shorter wavelengths, although the 0 .fwdarw. 0' transition may even lie at longer wavelengths than in the resp. sym. cyanine. The solvent may shift the symmetry of the dyes in merocyanines more towards the C2v or more towards the C.sigma. symmetry and thus also cause shifts of the absorption max. of the enveloping curve which need not be identical with shifts of the 0 .fwdarw. 0' transition.

IT 23786-72-3

(spectrum of, Franck-Condon factor in relation to electronic)

RN 23786-72-3 ZCAPLUS

CN Boron, [(1,2-dihydro-2,2'-methylidinediquinolinate)(1-)]difluoro-(8CI) (CA INDEX NAME)



IT 23786-72-3

(spectrum of, Franck-Condon factor in relation to electronic)

=> file beilstein

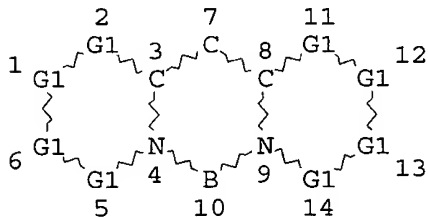
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L3 STR



VAR G1=C/N

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
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100.0% PROCESSED 151 ITERATIONS
SEARCH TIME: 00.00.04

6 ANSWERS

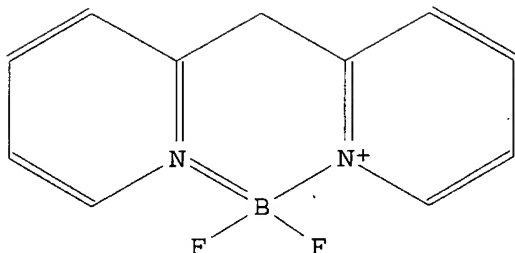
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L9 ANSWER 1 OF 6 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN):	5799690
Chemical Name (CN):	difluoro-(2,2'-methanediyl-bis-pyridine-N,N')-boron(1+); tetrafluoroborate
Lin. Struct. Formula (LSF):	C11H10BF2N2(1+)*BF4(1-)
Fragm. Molec. Formula (FMF):	C11 H10 B F2 N2 , B F4
Molecular Formula (MF):	C11 H10 B F2 N2 . B F4
Molecular Weight (MW):	219.02, 86.80
Fragment BRN (FBRN):	5793777, 3587364
Lawson Number (LN):	32713
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	5050294
Tautomer ID (TAUTID):	5487573
Beilstein Citation (BSO):	5-27
Entry Date (DED):	1993/05/06
Update Date (DUPD):	1996/08/08

CM 1

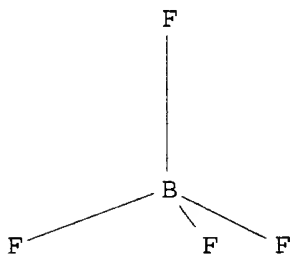
FBRN 5793777
FMF C11 H10 B F2 N2



CM 2

FBRN 3587364

FMF B F4



Fragment Notes:

Unknown location for Localized Charge of (-1)

Field Availability:

Code	Name	Occurrence
=====		
BRN	Beilstein Records	1
CN	Chemical Name	1
LSF	Linearized Structure Formula	1
FMF	Fragment Molecular Formula	2
MF	Molecular Formula	1
FW	Formular Weight	2
FBRN	Fragment BRN	2
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1

NMR Nuclear Magnetic Resonance 1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value (MP) (Cel)	Solvent (.SOL)	Ref.
172 - 173	aq. ethanol	1

Reference(s):

1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257

Nuclear Magnetic Resonance:

NMR

Description (.KW):	Chemical shifts
Nucleus (.NUC):	1H
Reference(s):	
1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257	

Reaction:

RX

Reaction ID (.ID):	1450691
Reactant BRN (.RBRN):	984585
Reactant (.RCT):	difluoro-(1',2'-dihydro-2,2'-methanylylidene-bis-pyridinato-N,N')-boron
Product BRN (.PBRN):	5799690
Product (.PRO):	difluoro-(2,2'-methanediyl-bis-pyridine-N,N')-boron(1+); tetrafluoroborate
No. of React. Details (.NVAR):	1

Reaction Details:

RX

Reaction RID (.RID):	1450691.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	HB ₄ F ₄
Solvent (.SOL):	ethanol
Reference(s):	
1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10,	

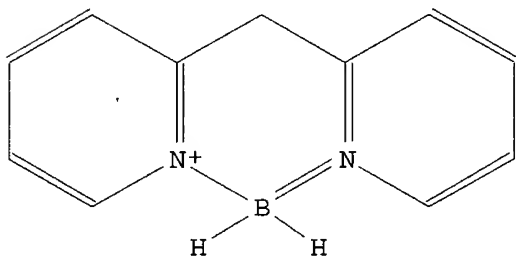
<1973>, 255-257

L9 ANSWER 2 OF 6 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 5799462
Chemical Name (CN): dihydrido-(2,2'-methanediyl-bis-pyridine-N,N')-boron(1+); hexafluorophosphate
Lin. Struct. Formula (LSF): C11H12BN2(1+)*F6P(1-)
Fragm. Molec. Formula (FMF): C11 H12 B N2 , F6 P
Molecular Formula (MF): C11 H12 B N2 . F6 P
Molecular Weight (MW): 183.04, 144.96
Fragment BRN (FBRN): 3965752, 3587827
Lawson Number (LN): 32713
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 5051577
Tautomer ID (TAUTID): 5488519
Beilstein Citation (BSO): 5-27
Entry Date (DED): 1993/05/06
Update Date (DUPD): 1996/08/08

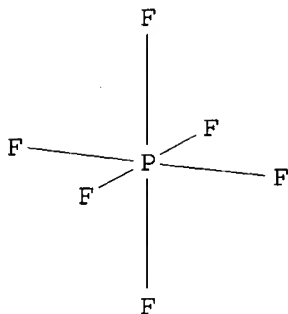
CM 1

FBRN 3965752
FMF C11 H12 B N2



CM 2

FBRN 3587827
FMF F6 P



Fragment Notes:

Unknown location for Localized Charge of (-1)

Field Availability:

Code	Name	Occurrence
=====	=====	=====
BRN	Beilstein Records	1
CN	Chemical Name	1
LSF	Linearized Structure Formula	1
FMF	Fragment Molecular Formula	2
MF	Molecular Formula	1
FW	Formular Weight	2
FBRN	Fragment BRN	2
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
=====	=====	=====
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value	Solvent	Ref.	Note
(MP)	(.SOL)		

(Cel)			
220 - 222	H2O	1	1

Reference(s):

1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257

Notes(s):

1. 50

Nuclear Magnetic Resonance:

NMR

Description (.KW):	Chemical shifts
Nucleus (.NUC):	1H
Reference(s):	
1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257	

Infrared Spectrum:

Descript	Ref.
ion	
(.KW)	
Bands	1

Reference(s):

1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257

Reaction:

RX

Reaction ID (.ID):	1275957
Reactant BRN (.RBRN):	5799608
Reactant (.RCT):	2,2'-methanediyl-bis-pyridine; bis-tetrafluoroborate
Product BRN (.PBRN):	5799462
Product (.PRO):	dihydrido-(2,2'-methanediyl-bis- pyridine-N,N')-boron(1+); hexafluorophosphate
No. of React. Details (.NVAR):	1

Reaction Details:

RX

Reaction RID (.RID):	1275957.1
Reaction Classification (.CL):	Preparation
Other Conditions (.COND):	(i) LiBH ₄ , (ii) aq. NH ₄ PF ₆
Note(s) (.COM):	Multistep reaction

Reference(s):

1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257

Reaction:

RX

Reaction ID (.ID): 8435696
Reactant BRN (.RBRN): 5799462
Reactant (.RCT): dihydrido-(2,2'-methanediyl-bis-pyridine-N,N')-boron(1+); hexafluorophosphate

No. of React. Details (.NVAR): 1

Reaction Details:

RX

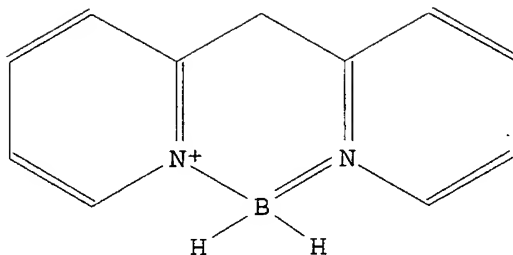
Reaction RID (.RID): 8435696.1
Reaction Classification (.CL): Chemical behaviour (half reaction)
Reference(s):
1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257

L9 ANSWER 3 OF 6 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 5797788
Chemical Name (CN): dihydrido-(2,2'-methanediyl-bis-pyridine-N,N')-boron(1+); iodide
Lin. Struct. Formula (LSF): C11H12BN2(1+)*I(1-)
Fragm. Molec. Formula (FMF): C11 H12 B N2 , I
Molecular Formula (MF): C11 H12 B N2 . I
Molecular Weight (MW): 183.04, 126.90
Fragment BRN (FBRN): 3965752, 3587184
Lawson Number (LN): 32713
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 5045897
Tautomer ID (TAUTID): 5481519
Beilstein Citation (BSO): 5-27
Entry Date (DED): 1993/05/06
Update Date (DUPD): 1996/08/08

CM 1

FBRN 3965752
FMF C11 H12 B N2



CM 2

FBRN 3587184

FMF I

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
LSF	Linearized Structure Formula	1
FMF	Fragment Molecular Formula	2
MF	Molecular Formula	1
FW	Formular Weight	2
FBRN	Fragment BRN	2
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value (MP) (Cel)	Solvent (.SOL)	Ref.
79 - 81	ethanol	1

Reference(s):

1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257

Nuclear Magnetic Resonance:

NMR

Description (.KW):	Chemical shifts
Nucleus (.NUC):	1H
Reference(s):	
1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257	

Infrared Spectrum:

Descript ion (.KW)	Ref.
Bands	1

Reference(s):

1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257

Reaction:

RX

Reaction ID (.ID):	928901
Reactant BRN (.RBRN):	120459
Reactant (.RCT):	2,2'-methanediyl-bis-pyridine
Product BRN (.PBRN):	5797788
Product (.PRO):	dihydrido-(2,2'-methanediyl-bis-pyridine-N,N')-boron(1+); iodide
No. of React. Details (.NVAR):	1

Reaction Details:

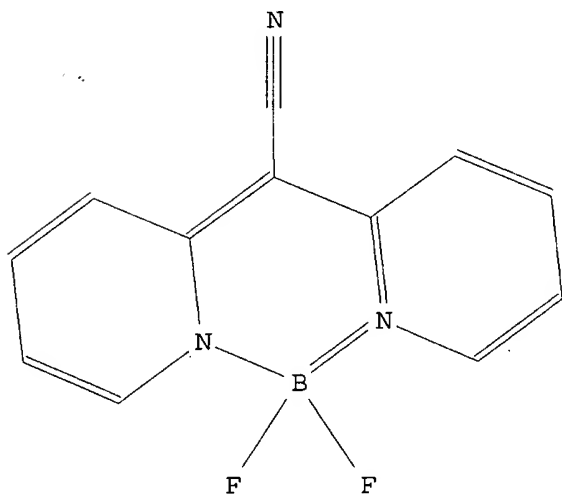
RX

Reaction RID (.RID):	928901.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	BH2I*Py
Reference(s):	
1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10,	

<1973>, 255-257

L9 ANSWER 4 OF 6 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 1000470
Chemical Name (CN): (di-pyridin-2-yl-acetonitrilato-N1',N1'')-difluoro-boron,
(1-difluoroboranyl-1H-pyridin-2-ylidene)-pyridin-2-yl-acetonitrile
Molec. Formula (MF): C12 H8 B F2 N3
Molecular Weight (MW): 243.02
Lawson Number (LN): 32739
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 958027
Tautomer ID (TAUTID): 970878
Beilstein Citation (BSO): 5-27
Entry Date (DED): 1988/11/29
Update Date (DUPD): 1996/08/08



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	2
MF	Molecular Formula	1
FW	Formular Weight	1

LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
FINFO	Further Information	1

Further Information:

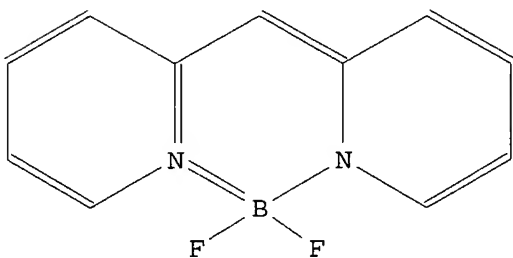
FINFO

Reference(s):

1. Scheibe et al., Z.Phys.Chem.(Munich), CODEN: ZPCFAX, 64, <1969>, 97

L9 ANSWER 5 OF 6 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN):	984585
Chemical Name (CN):	difluoro-(1',2'-dihydro-2,2'-methanylylidene-bis-pyridinato-N,N')-boron, 1'-difluoroboranyl-1',2'-dihydro-2,2'-methanylylidene-bis-pyridine
Molec. Formula (MF):	C11 H9 B F2 N2
Molecular Weight (MW):	218.01
Lawson Number (LN):	32713
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	874047
Tautomer ID (TAUTID):	877443
Beilstein Citation (BSO):	5-27
Entry Date (DED):	1988/11/29
Update Date (DUPD):	1996/08/08



Field Availability:

Code	Name	Occurrence
=====	=====	=====
BRN	Beilstein Records	1
CN	Chemical Name	2
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	2
UVS	UV and Visible Spectrum	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
=====	=====	=====
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value	Solvent	Ref.
(MP)	(.SOL)	
(Cel)		
=====	=====	=====
130	aq. ethanol	1

Reference(s):

1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257

Nuclear Magnetic Resonance:

NMR

Description (.KW):	Chemical shifts
Nucleus (.NUC):	19F
Reference(s):	
1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257	

NMR

Description (.KW):	Chemical shifts
Nucleus (.NUC):	1H
Reference(s):	
1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257	

UV and Visible Spectrum:

Description (.KW)	Ref.
=====+=====	
Absorption maxima	1

Reference(s):

1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257

Reaction:

RX

Reaction ID (.ID):	1275958
Reactant BRN (.RBRN):	5799608
Reactant (.RCT):	2,2'-methanediyl-bis-pyridine; bis-tetrafluoroborate
Product BRN (.PBRN):	984585
Product (.PRO):	difluoro-(1',2'-dihydro-2,2'- methanylylidene-bis-pyridinato-N,N')- boron
No. of React. Details (.NVAR):	1

Reaction Details:

RX

Reaction RID (.RID):	1275958.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	NaBH4
Temperature (.T):	190 - 200 Cel
Reference(s):	1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257

Reaction:

RX

Reaction ID (.ID):	1450691
Reactant BRN (.RBRN):	984585
Reactant (.RCT):	difluoro-(1',2'-dihydro-2,2'- methanylylidene-bis-pyridinato-N,N')- boron
Product BRN (.PBRN):	5799690
Product (.PRO):	difluoro-(2,2'-methanediyl-bis- pyridine-N,N')-boron(1+); tetrafluoroborate
No. of React. Details (.NVAR):	1

Reaction Details:

RX

Reaction RID (.RID):	1450691.1
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Reaction Classification (.CL): Preparation

Reagent (.RGT): HBF₄

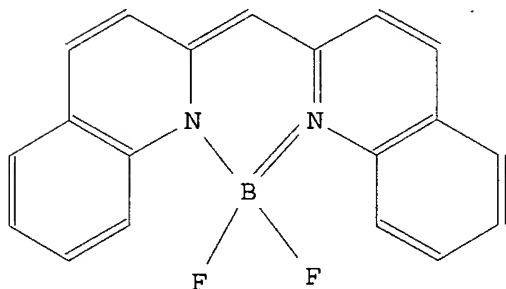
Solvent (.SOL): ethanol

Reference(s):

1. Douglass, J. et al., J.Heterocycl.Chem., CODEN: JHTCAD, 10, <1973>, 255-257

L9 ANSWER 6 OF 6 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 559019
Chemical Name (CN): difluoro-(1',2'-dihydro-2,2'-methanylylidene-bis-quinolinato-N,N')-boron, 1'-difluoroboranyl-1',2'-dihydro-2,2'-methanylylidene-bis-quinoline
Molec. Formula (MF): C₁₉ H₁₃ B F₂ N₂
Molecular Weight (MW): 318.13
Lawson Number (LN): 32717
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 525080
Tautomer ID (TAUTID): 509151
Beilstein Citation (BSO): 5-27
Entry Date (DED): 1988/11/28
Update Date (DUPD): 1996/08/08



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	2
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1

TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
FINFO	Further Information	1

Further Information:

FINFO

Reference(s):

1. Scheibe et al., Z.Phys.Chem.(Munich), CODEN: ZPCFAX, 64, <1969>, 97